Reduced fidelity susceptibility in the one-dimensional transverse field Ising model

Jian Ma,[1] Lei Xu,[1] and Xiaoguang Wang[1, *]

[1]*Zhejiang Institute of Modern Physics, Department of Physics,*
Zhejiang University, HangZhou 310027, P.R. China.
(Dated: August 13, 2008)

We study critical behaviors of the reduced fidelity susceptibility for two neighboring sites in the one-dimensional transverse field Ising model. It is found that the divergent behaviors of the susceptibility take the form of square of logarithm, in contrast with the global ground-state fidelity susceptibility which is power divergence. In order to perform a scaling analysis, we take the square root of the susceptibility and determine the scaling exponent analytically and the result is further confirmed by numerical calculations.

I. INTRODUCTION

Within the last few years, some concepts and tools in the field of quantum information science [1], such as entanglement and fidelity, have been introduced in the study of quantum phase transitions (QPTs) [2], which are described traditionally in terms of order parameters and symmetry breaking. However, without *a priori* knowledge of the order parameter, when a system undergoes QPT, its ground state will change dramatically. Since the definition of fidelity is the overlap between two quantum states, it's natural to introduce it in the field of QPTs. The most studied fidelity is the global ground state fidelity [3–21], which is an overlap between two ground states with a slight change of the parameters. Therefore, to avoid the arbitrariness of the small change in numerical computation, Zanardi et al. introduced the Riemannian metric tensor [8, 9], while You et al. suggested the fidelity susceptibility [10], which is an effective tool to study the critical properties.

So far, in most works, people have concerned with the global ground state fidelity. We note that as far as in Ref [22] the authors have introduced a reduced fidelity which is defined as the trace of the product of two matrices. This definition is not rigorous in quantum-information theory, and they require one of the density matrices to be a pure state to agree with the rigorous mixed state fidelity [29]. While in this paper, the reduced fidelity we used is defined rigorously in quantum-information theory and is studied in [14, 23–26]. It has been shown that the reduced fidelity susceptibility (RFS) is an efficient indicator of QPTs.

In this paper, we study the scaling and critical behaviors of the RFS of two neighboring sites in the famous one-dimensional (1D) transverse field Ising model (TFIM). We note that the quantum critical properties of some other quantities like concurrence [27] and von Neumann entropy [28], and the global ground state fidelity

susceptibility [11] have been studied in this model. However, the scaling and critical behaviors of them are quite different from the RFS for two neighboring sites . It's found that the scaling and critical behaviors of the RFS take the form of square of logarithm as $(\ln N)^2$ for finite-size system and $(\ln|\lambda - 1|)^2$ (N is the total number of spins and external parameter $\lambda = 1$ is the critical point) in the thermodynamic limit, in contrast with the global fidelity susceptibility [11], which takes the form of N and $|1 - \lambda|^{-1}$, respectively. The different scaling and critical behaviors lead to a different finite-size scaling analysis, and for RFS we have to take its square root which is logarithmic divergent to carry out the scaling analysis.

The paper is organized as follows. In Sec. II, we briefly review some concepts in fidelity and its susceptibility, and then we introduce a general formula of the RFS derived in [25]. In Sec. III, the scaling and critical behaviors are obtained analytically for both finite-size and thermodynamic limit, respectively. Then, using the square root of the RFS, we perform a finite-size scaling analysis. The scaling exponent is determined analytically, and is confirmed numerically.

II. REDUCED FIDELITY SUSCEPTIBILITY

Firstly, let us review some concepts in fidelity susceptibility. The Hamiltonian of a quantum system undergoing QPTs can be written as

$$H(h) = H_0 + hH_I, \tag{1}$$

where H_I is supposed to be the driving term with a control parameter h. The fidelity between two RDMs of the ground state $\rho \equiv \rho(h)$ and $\tilde{\rho} \equiv \rho(h + \delta)$ is defined as [29]

$$F(h, \delta) = \text{tr}\sqrt{\rho^{1/2}\tilde{\rho}\rho^{1/2}}. \tag{2}$$

The fidelity susceptibility is given by [4, 10]

$$\chi = \lim_{\delta \to 0} \frac{-2\ln F}{\delta^2}, \tag{3}$$

*Electronic address: xgwang@zimp.zju.edu.cn

therefore we have $F \simeq 1 - \chi \delta^2 / 2$.

In this paper, we study the RFS of two neighboring sites, and the RDM is block-diagonal as $\rho = \varrho_1 \oplus \varrho_2$ due to the specific symmetries in the 1D TFIM, and ϱ_1, ϱ_2 are 2×2 matrices. In [25], we have derived general formulas of RFS for density matrix of block-diagonal as $\rho = \oplus_{i=1}^n \varrho_i$, where ϱ_i's are 2×2 matrices. However, in this work the density matrix satisfies $\det \varrho_i \neq 0$ and $\mathrm{tr} \varrho_i \neq 0$ $(i = 1, 2)$, then we give the formula under such case as follows [25],

$$\chi_i = \frac{1}{4 \mathrm{tr} \varrho_i} \left\{ (\mathrm{tr} \varrho_i')^2 - 4 \det \varrho_i' + \frac{[\partial_h \det (\varrho_i)]^2}{\det (\varrho_i)} \right\}, \quad (4)$$

where $\varrho' \equiv \partial_h \varrho$, and χ_i is the 'susceptibility' for block ϱ_i. From the above formula we can see that the RFS is only depends upon to the first derivatives of the matrix elements.

III. SCALING AND CRITICAL BEHAVIORS OF RFS IN 1D TFIM

The Hamiltonian of the 1D TFIM reads

$$H_I = - \sum_{j=-M}^M \left[\lambda \sigma_j^x \sigma_{j+1}^x + \sigma_j^z \right], \quad (5)$$

where σ_j^α $(\alpha = x, y, z)$ is a Pauli matrix at site j, λ is the Ising coupling constant in units of the transverse field, and periodic boundary conditions $(\sigma_{-M} = \sigma_M)$ are assumed. The total spins are $N = 2M + 1$, and in this

paper we consider N is even, therefore M is half odd integer. As is well known, there is a critical point exactly at $\lambda_c = 1$ in the thermodynamic limit. The transition in this model is of order to disorder type due to the competition between the Ising coupling and the external magnetic field. For $\lambda < \lambda_c$, the ground state of the system is paramagnetic, while for $\lambda > \lambda_c$ the strong Ising coupling introduces a magnetic long-range order of the order parameter $\langle \sigma^x \rangle$ to the ground state.

The RDM of two neighboring sites takes the form of [30]

$$\rho_{i,i+1} = \begin{pmatrix} u_+ & z_- & 0 & 0 \\ z_- & u_- & 0 & 0 \\ 0 & 0 & w & z_+ \\ 0 & 0 & z_+ & w \end{pmatrix}, \quad (6)$$

in the basis $\{| \uparrow\uparrow \rangle, | \downarrow\downarrow \rangle, | \uparrow\downarrow \rangle, | \downarrow\uparrow \rangle\}$ with $| \uparrow \rangle$ and $| \downarrow \rangle$ spin up and down. The matrix elements are

$$u_\pm = \frac{1}{4} \left(1 \pm 2\langle \sigma^z \rangle + \langle \sigma_0^z \sigma_1^z \rangle \right),$$
$$w = \frac{1}{4} \left(1 - \langle \sigma_0^z \sigma_1^z \rangle \right),$$
$$z_\pm = \frac{1}{4} \left(\langle \sigma_0^x \sigma_1^x \rangle \pm \langle \sigma_0^y \sigma_1^y \rangle \right). \quad (7)$$

where the translation invariance of the 1D TFIM is considered, and we set $i = 0$ for convenience in what follows. From Eqs. (4) and (6), the RFS can be written explicitly with these matrix elements as

$$\chi = \frac{1}{4 (u_+ + u_-)} \left[(\partial_\lambda u_+ - \partial_\lambda u_-)^2 + 4 (\partial_\lambda z_-)^2 + \frac{(u_- \partial_\lambda u_+ + u_+ \partial_\lambda u_- - 2 z_- \partial_\lambda z_-)^2}{u_+ u_- - z_-^2} \right]$$
$$+ \frac{1}{2w} \left[(\partial_\lambda z_+)^2 + \frac{(w \partial_\lambda w - z_+ \partial_\lambda z_+)^2}{w^2 - z_+^2} \right]. \quad (8)$$

The following discussions of critical behaviors of the RFS is based on this equation.

The Hamiltonian could be diagonalized by using Jordan-Wigner, Fourier and Bogoliubov transformation sequently (see [2]), and the mean magnetization in the ground state is given by [31]

$$\langle \sigma^z \rangle = \frac{1}{N} \sum_{q=-M}^M \frac{1 - \lambda \cos \phi_q}{\omega_{\phi_q}}, \quad (9)$$

where ω_{ϕ_q} is the dispersion relation,

$$\omega_{\phi_q} = \sqrt{1 + \lambda^2 - 2\lambda \cos \phi_q},$$
$$\phi_q = 2\pi q / N, \quad (10)$$

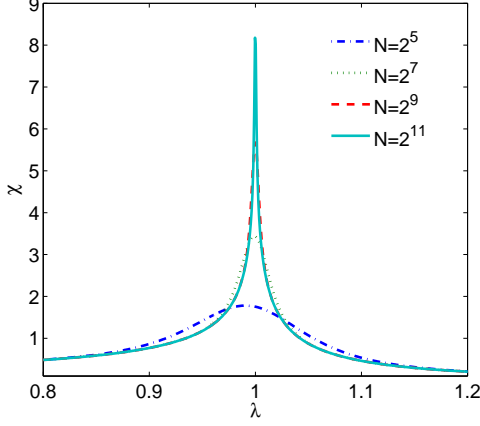with q half odd integer. The neighboring two-point correlation functions are calculated as [32]

FIG. 1: RFS as a function of λ for various system sizes. The positions of the peaks approach to the critical point at $\lambda = 1$ as increase with system sizes.

$$\langle \sigma_0^x \sigma_1^x \rangle = \frac{1}{N} \sum_{q=-M}^{M} \frac{\lambda - \cos \phi_q}{\omega_{\phi_q}},$$

$$\langle \sigma_0^y \sigma_1^y \rangle = \frac{1}{N} \sum_{q=-M}^{M} \frac{\lambda \cos (2\phi_q) - \cos \phi_q}{\omega_{\phi_q}},$$

$$\langle \sigma_0^z \sigma_1^z \rangle = \langle \sigma^z \rangle^2 - \langle \sigma_0^x \sigma_1^x \rangle \langle \sigma_0^y \sigma_1^y \rangle. \quad (11)$$

It's known that the most important themes in critical phenomena are scaling and universality. For a finite system, there are no singularities unless the ground state level crossing occurs. In the following, we will calculate the mean magnetization, the correlation functions and their first derivatives, and get the finite-size scaling and critical behaviors of RFS.

A. Finite-size scaling behavior of RFS

The numerical results of the RFS for a finite-size system are shown in Fig. 1, from which we can see that the peaks become sharper and sharper as the system size increases, and their locations approach to the critical point at the same time. It's expected that there will be singular at λ_c if N is infinite. Then to study the scaling behavior of RFS, we define its maximum over λ as χ_m with the location λ_m. For a finite-size system, $\lambda_m \neq \lambda_c$, and yet if N is large enough, λ_m is so close to λ_c that it's a good approximation for us to use $\lambda_m = \lambda_c$ in computing χ_m. The summations in Eqs. (9) and (11) converge quickly as N increases, which means for large N, the summation can be replaced by the integral as

$$\lim_{N \to \infty} \frac{1}{N} \sum_{q=-M}^{M} \longrightarrow \frac{1}{2\pi} \int_{-\pi}^{\pi} d\phi. \quad (12)$$

Then it's easy to evaluate the integrals and get

$$\langle \sigma^z \rangle|_{\lambda=1} = \frac{2}{\pi}, \qquad \langle \sigma_0^x \sigma_1^x \rangle|_{\lambda=1} = \frac{2}{\pi},$$

$$\langle \sigma_0^y \sigma_1^y \rangle|_{\lambda=1} = -\frac{2}{3\pi}, \qquad \langle \sigma_0^z \sigma_1^z \rangle|_{\lambda=1} = \frac{16}{3\pi^2}. \quad (13)$$

However, the first derivatives of the above quantities are divergent with respect to N at λ_c, and we have

$$\frac{d\langle \sigma^z \rangle}{d\lambda}\bigg|_{\lambda=1} = -\frac{1}{2N} \sum_{q=-M}^{M} \left| \frac{\cos^2 (\phi_q/2)}{\sin (\phi_q/2)} \right| \simeq -\frac{1}{\pi} \ln N,$$

$$\frac{d\langle \sigma_0^x \sigma_1^x \rangle}{d\lambda}\bigg|_{\lambda=1} = \frac{1}{2N} \sum_{q=-M}^{M} \left| \frac{\cos^2 (\phi_q/2)}{\sin (\phi_q/2)} \right| \simeq \frac{1}{\pi} \ln N,$$

$$\frac{d\langle \sigma_0^y \sigma_1^y \rangle}{d\lambda}\bigg|_{\lambda=1} = \frac{1}{4N} \sum_{q=-M}^{M} \frac{\cos (2\phi_q) + \cos \phi_q}{|\sin (\phi_q/2)|} \simeq \frac{1}{\pi} \ln N. \quad (14)$$

The main contribution to the above expressions in the large-N limit arises from the summation around the zero point of $\sin(\phi_q/2)$, since

$$\frac{1}{N} \sum_{q \in S} \frac{1}{|\phi_q|} \simeq \frac{1}{\pi} \ln N, \quad (15)$$

where S represents the singular area. Immediately, with the help of Eqs. (4) and (11), we get

$$\frac{d\langle \sigma_0^z \sigma_1^z \rangle}{d\lambda}\bigg|_{\lambda=1} \simeq -\frac{16}{3\pi^2} \ln N. \quad (16)$$

The matrix elements and their derivatives could be evaluated by inserting the above results into Eq. (7). Here we should specifically consider $\partial_\lambda z_- = \partial_\lambda (\langle \sigma_0^x \sigma_1^x \rangle - \langle \sigma_0^y \sigma_1^y \rangle)/4$, the divergent behaviors of $\partial_\lambda \langle \sigma_0^x \sigma_1^x \rangle$ and $\partial_\lambda \langle \sigma_0^y \sigma_1^y \rangle$ at λ_c are both $(\ln N)/\pi$, while their difference is convergent and could be integrated as a constant:

$$\frac{dz_-}{d\lambda}\bigg|_{\lambda=1} = \frac{1}{3\pi}. \quad (17)$$

Then, with Eq. (8), we get the divergent form of χ_m with respect to N as

$$\chi_m (N) \simeq A_1 (\ln N + c_1)^2 + c_2, \quad (18)$$

where c_1, c_2 are constants that could not be determined analytically, and the coefficient

$$A_1 = \frac{27\pi^4 - 144\pi^2 - 1024}{\pi^2 (9\pi^2 + 32)(3\pi^2 - 32) + 4096}$$
$$\simeq 0.1485. \quad (19)$$

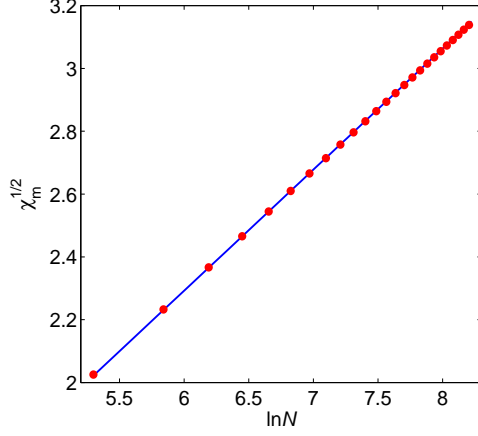To perform a finite-size scaling analysis, we should find the logarithmic divergent quantity, and the above result

FIG. 2: Square of the maximum RFS over λ as a function of N. The red dots are numerical results and the slope of the solid line is $\sqrt{A_1}$.
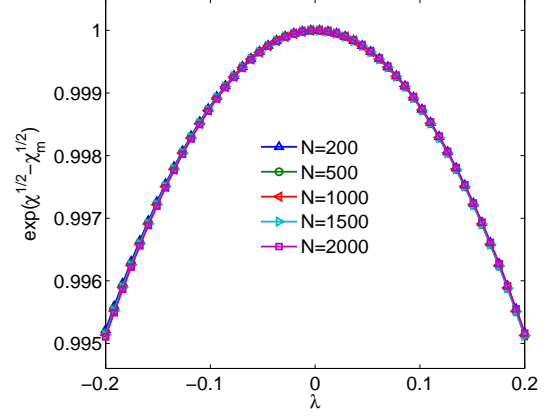

FIG. 3: Finite-size scaling analysis is performed. The RFS as a function of system size and coupling, collapses on a single curve for various system sizes.

suggests us to take the square root of χ_m for large N to get the logarithmic divergent form as

$$\chi_m (N)^{1/2} \simeq \sqrt{A_1} \ln N + \text{const.} \qquad (20)$$

To confirm this, we compute $\chi_m^{1/2}$ numerically, and the result is shown in Fig. 2, from which we can see that the slope is excellently consistent with $\sqrt{A_1}$, while the linear relation is obvious for not large N because c_2 is small with numerical computation. However the maximum global ground state fidelity susceptibility S_m is of a different scaling form as $\ln S_m = 2 \ln N + \text{const}$ [11], thus $\ln S_m$ but not S_m will exhibit similar scaling behavior with $\chi_m^{1/2}$ at the critical point.

B. Critical behavior of RFS in the thermodynamic limit

In the thermodynamic limit the total spin N is infinite, then the summations can be replaced by the integrals (12) and are evaluated as:

$$
\begin{aligned}
\langle \sigma^z \rangle =& \frac{1-\lambda}{\pi} \mathrm{K}(k) + \frac{1+\lambda}{\pi} \mathrm{E}(k), \\
\langle \sigma_0^x \sigma_1^x \rangle =& \frac{\lambda-1}{\pi} \mathrm{K}(k) + \frac{1+\lambda}{\pi} \mathrm{E}(k), \\
\langle \sigma_0^y \sigma_1^y \rangle =& \frac{1}{3\pi\lambda} \big[\mathrm{K}(k)(\lambda-1)(2\lambda^2+1) \\
& - \mathrm{E}(k)(\lambda+1)(2\lambda^2-1) \big], \qquad (21)
\end{aligned}
$$

where $\mathrm{K}(k)$ is the complete elliptic integral of the first kind and $\mathrm{E}(k)$ is the elliptic integral of the second kind with $k = 2\sqrt{\lambda}/(1+\lambda)$. Therefore the critical behavior of the RFS is determined by the elliptical integrals. At λ_c, we have $k_c = 2\sqrt{\lambda_c}/(1+\lambda_c) = 1$, and $\mathrm{E}(1) = 1$, while

$\mathrm{K}(k)$ is divergent as $k \to 1$, its asymptotic behavior is

$$\mathrm{K}(k) \simeq \ln \frac{1}{\sqrt{1-k^2}} = \ln \frac{1}{|1-\lambda|}, \qquad (22)$$

from which we have $\mathrm{K}(k_c)(1-\lambda_c) = 0$. Then, obviously, at the critical point, with the above analysis we get the same results with (13) in the previous subsection.

However, their derivatives are singular at $\lambda = 1$. We take $\langle \sigma^z \rangle$ for example,

$$\frac{d\langle \sigma^z \rangle}{d\lambda} = \frac{\lambda+1}{\pi\lambda} \mathrm{E}(k) - \frac{\lambda^2+1}{\pi\lambda(\lambda+1)} \mathrm{K}(k), \qquad (23)$$

where we have used the following relations

$$
\begin{aligned}
\frac{d\mathrm{K}(k)}{dk} &= \frac{\mathrm{E}(k)}{k} - \frac{\mathrm{K}(k)}{k}, \\
\frac{d\mathrm{E}(k)}{dk} &= \frac{\mathrm{E}(k)}{(1-k^2)k} - \frac{\mathrm{K}(k)}{k}. \qquad (24)
\end{aligned}
$$

Then as λ approaches to λ_c, $\mathrm{E}(k)$ converges quickly to 1, and with Eq. (22) we get

$$\frac{d\langle \sigma^z \rangle}{d\lambda} \simeq -\frac{1}{\pi} \ln \frac{1}{|1-\lambda|}, \qquad (25)$$

which is logarithmic divergent as $\lambda \to \lambda_c$. The derivatives of the rest correlation functions are

$$
\begin{aligned}
\frac{d\langle \sigma_0^x \sigma_1^x \rangle}{d\lambda} &\simeq \frac{1}{\pi} \ln \frac{1}{|1-\lambda|}, \\
\frac{d\langle \sigma_0^y \sigma_1^y \rangle}{d\lambda} &\simeq \frac{1}{\pi} \ln \frac{1}{|1-\lambda|}, \\
\frac{d\langle \sigma_0^z \sigma_1^z \rangle}{d\lambda} &\simeq -\frac{16}{3\pi^2} \ln \frac{1}{|1-\lambda|}, \qquad (26)
\end{aligned}
$$

where the logarithmic divergent terms come from the elliptic integral $\mathrm{K}(k)$. It's noticed that the coefficients of

the logarithmic terms are the same with those in the previous subsection for a finite-size system. Then we get a similar divergent form of χ as

$$\chi(\lambda) \simeq A_2 \left(\ln \frac{1}{|1-\lambda|} + d_1 \right)^2 + d_2,$$

where $A_2 = A_1$, and d_1, d_2 are constants that could not be determined analytically.

As we have derived in the above, the divergent form of the RFS around the critical point is $(\ln N)^2$ for finite system and $(\ln|1-\lambda|)^2$ in the thermodynamic limit. In order to make a finite size scaling analysis, it's feasible for us to use the square root of the RFS, which is logarithmic divergent, and according to the scaling ansatz [33], the square root of RFS is a function of $N^\nu(\lambda - \lambda_m)$, which behaves as $\chi(\lambda_m, N)^{1/2} - \chi(\lambda, N)^{1/2} \sim Q[N^\nu(h-h_m)]$, where $Q(x) \propto \ln(x)$ for large x. This function is universal and does not depend on system size N. Since $A_2 = A_1$, we determine the scaling exponent $\nu = 1$ which is the same with the concurrence [27] and the global ground state fidelity susceptibility [11], and is confirmed numerically shown in Fig. 3.

IV. CONCLUSION

In summary, we have studied the scaling and critical behaviors of the RFS for two neighboring sites in the 1D TFIM. We found that the divergent behaviors of the RFS take the form of $(\ln N)^2$ for finite-size system and $(\ln|\lambda - 1|)^2$ in the thermodynamic limit, which are distinct from other quantities like the global ground state fidelity susceptibility [11], concurrence [27] and entanglement entropy [28]. Then we use the square root of the RFS which is logarithmic divergent to carry out a finite-size scaling analysis. The scaling exponent is determined analytically, and is confirmed numerically. It's shown that, the RFS undergoes singularity around the critical point, thus indicate that the RFS can be used to characterize the QPTs.

V. ACKNOWLEDGEMENTS

[1] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information* (Cambidge University Press, Cambidge, U.K., 2000).
[2] S. Sachdev, *Quantum Phase Transitions* (Cambidge University Press, Cambidge, U.K.,1999).
[3] H. T. Quan, Z. Song, X. F. Liu, P. Zanardi, and C. P. Sun, Phys. Rev. Lett. **96**, 140604 (2006).
[4] P. Zanardi and N. Paunković, Phys. Rev. E **74**, 031123 (2006).
[5] P. Buonsante and A. Vezzani, Phys. Rev. Lett. **98**, 110601 (2007).
[6] P. Zanardi, M. Cozzini, and P. Giorda, J. Stat. Mech. **2**, L02002 (2007).
[7] M. Cozzini, P. Giorda, and P. Zanardi, Phys. Rev. B **75**, 014439 (2007).
[8] L. C. Venuti and P. Zanardi, Phys. Rev. Lett. **99**, 095701 (2007).
[9] Paolo Zanardi and Marco Cozzini, Phys. Rev. Lett. **99**, 100603 (2007).
[10] W.-L. You, Y.-W. Li, and S.-J. Gu, Phys. Rev. E **76**, 022101 (2007).
[11] S. Chen, L. Wang, Y. Hao, and Y. Wang, Phys. Rev. A **77**, 032111 (2008).
[12] H. Q. Zhou and J. P. Barjaktarevic, arXiv:cond-mat/0701608 (2007).
[13] H. Q. Zhou, J. H. Zhao, and B. Li, arXiv:0704.2940 (2007).
[14] H. Q. Zhou, arXiv:0704.2945 (2007).
[15] S. J. Gu, H. M. Kwok, W. Q. Ning, and H. Q. Lin, arXiv:0706.2495 (2007).
[16] S. Chen, L. Wang, S.-J. Gu, and Y. Wang, Phys. Rev. E **76**, 061108 (2007).
[17] W. Q. Ning, S. J. Gu, C. Q. Wu, and H. Q. Lin, J. Phys.: Condens. Matter **20**, 235236 (2008).
[18] H.-M. Kwok, W.-Q. Ning, S.-J. Gu, and H.-Q. Lin, arXiv:0710.2581v1 (2008).
[19] M.-F. Yang, Phys. Rev. B **76**, 180403 (2007).
[20] J.-H. Zhao and H.-Q. Zhou, arXiv:0803.0814 (2008).
[21] S. Yang, S.-J. Gu, C.-P. Sun, and H.-Q. Lin, arXiv:0803.1292 (2008).
[22] Marko Žnidarič and Tomaž Prosen, J. Phys. A **36**, 2463 (2003).
[23] T. Gorin, T. Prosen, T. H. Seligman, and M. Znidaric, Phys. Rep. **435**, 33 (2006).
[24] N. Paunkovic, P. D. Sacramento, P. Nogueira, V. R. Vieira, and V. K. Dugaev, Phys. Rev. A **77**, 052302 (2008).
[25] J. Ma, L. Xu, H.-N. Xiong, and X. Wang, arXiv:0805.4062v1 (2008).
[26] H.-M. Kwok, C.-S. Ho, and S.-J. Gu, arXiv:0805.3885v2 (2008).
[27] A. Osterloh, L. Amico, G. Falci, and R. Fazio, Nature **416**, 608 (2002).
[28] S.-Q. Su, J.-L. Song, and S.-J. Gu, Phys. Rev. A **74**,

032308 (2006).

[29] A. Uhlmann, Rep. Math. Phys. **9**, 272 (1976).

[30] X. Wang and K. Mølmer, Eur. Phys. J. D **18**, 385 (2002).

[31] E. Barouch and B. M. McCoy, Phys. Rev. A **2**, 1075 (1970).

[32] E. Barouch and B. M. McCoy, Phys. Rev. A **3**, 786 (1971).

[33] M. N. Barber, *Phase Transition and Critical Phenomena*, (Academic, London, 1983), Vol.8, pp. 149-259.